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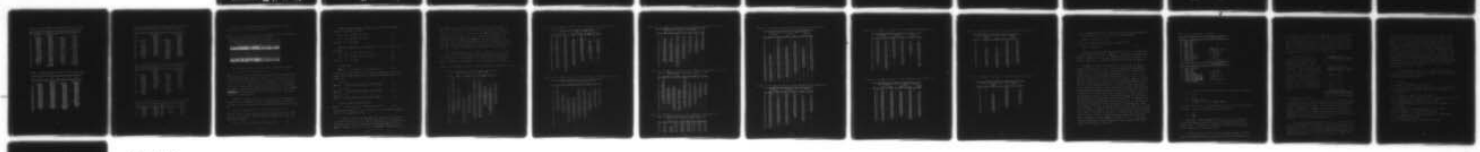

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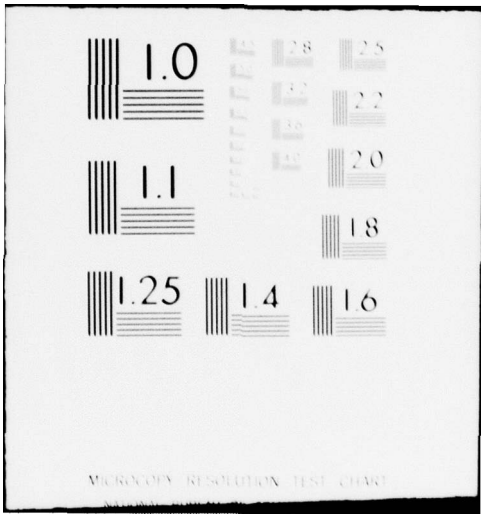
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FOREIGN TECHNOLOGY DIVISION

THE ROTATION STRUCTURE OF THE EMISSION SPECTRUM OF THE SULFUR MOLECULE S_2

by

S. Meiring Naude

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The Rotation Structure of the Emission Spectrum of the Sulfur Molecule S_2

S. Meiring Naudé

Summary of Contents

The emission spectrum of the S_2 molecule was recorded with a Geissler discharge tube at the third and fourth order of a 6.4 m Paschen grid. In the fourth order, the dispersion was 0.57 Å per mm. The analysis of the following bands will be reported here: (1.14) at 4433.6 Å, (2.17) at 4747.6 Å, (3.17) at 4651.3 Å, (3.19) at 4937.2 Å, (4.19) at 4842.2 Å, (4.22) at 5309.9 Å, (5.22) at 5193.7 Å, (5.23) at 5359.7 Å, (6.23) at 5249.8 Å, (6.25) at 5596.1 Å, (7.25) at 5472.5 Å, (7.27) at 5840.2 Å, and (8.27) at 5709.6 Å. In the stronger bands, three R branches and three P branches were discovered. The structure of the bands is entirely analogous to that of the Schumann-Runge O_2 bands. The S_2 bands are to be attributed to a $3\Sigma_u^- \rightarrow 3\Sigma_g^-$-transition. The values of the constants B_e' and B_e'' are 0.2219 and 0.2956 cm^{-1} respectively. The nuclear distance of the higher state is $r_e = 2.180 \cdot 10^{-8}$ cm and of the lower state $r_e'' = 1.893 \cdot 10^{-8}$ cm. It was determined that the rotation levels with odd K-values are absent in the upper state, and those with even quantum numbers in the lower state. From this fact it can be concluded that the S^{32} atom has no nuclear spin.

I. Introduction

Sulfur is characterized by an extended emission spectrum of the S_2 molecule, which stretches from 6200 to 2400 Å. The vibrational structure of this spectral system has already been the subject of a number of studies, for example by Rosen [1], Christy and Naudé [2], and by Fowler and Vaidya [3]. Christy and Naudé found that the vibration differences of the higher state of the S_2 molecule or the $\Delta G'$ values are significantly distorted (see Table 1). This result was confirmed by Fowler and Vaidya. They were able through intensive study of the flame spectrum of CS_2 to conduct a more thorough vibrational analysis of the S_2 bands, and

Table 1 is based on their efforts.

Table 1: $\Delta G'$ values of the S_2 bands

v' =	0	1	2	3	4	5	6	7	8	9	10
$\Delta G'$ =	447	415	433	397	417	388	402	391	383	379	cm^{-1}

(The table is to be read as follows: $\Delta G'$ between v'=0 and v'=1 is 447 cm^{-1}, etc.)

From the irregular behavior of the $\Delta G'$ values, large disturbances in the rotational structure of the bands are to be expected. Olsson [4] succeeded in obtaining a satisfactory rotational analysis of the (1.4), (2.4), (1.3), (2.3), (3.3), (2.2) and (3.2) bands in absorption. From this work, it could already be seen that the disturbances of the $\Delta G'$ values also have an effect on the rotational structure. However, it is not possible to investigate the disturbances of the rotation structure precisely in absorption, since it is impossible to obtain precise measurements of the lines in the vicinity of the band head. For this reason the rotation analysis of the (1.14), (1.15), (2.16), (2.17), (3.17), (3.18) and (3.19) bands was undertaken in emission by Naudé [5]. This work also served to confirm the vibration analysis of Fowler and Vaidya and the rotation analysis of Olsson.

In this work [5], many unexplained observations arose, no doubt associated with the disturbed $\Delta G'$ values. In order to clarify these phenomena, the (4.19), (4.22), (5.22), (5.23), (6.23), (6.25), (7.25), (7.27) and (8.27) bands were also analyzed. Although the disturbances have not yet been explained, it nevertheless seems important that the results obtained be published, so that the puzzling disturbances in the S_2 bands may be tracked down. Because the work cited is not very accessible, the data of the (1.14), (2.17), (3.17) and (3.19) bands will be reviewed, and the $\Delta_2 F_1'$, $\Delta_2 F_2'$ and $\Delta_2 F_3'$ will be compared with those of Olsson.

II. Experiment

The tube shown in Figure 1 served as the light source for the S_2 spectrum. The sulfur was purified by quadruple slow vacuum distillation of pure flowers of sulfur, and then placed in the container S of the figure. The electrical discharge between the two electrodes occurred through a capillary tube of 3 mm inside diameter. In this way the light of discharge was concentrated, and exited through a quartz window at one end of the capillary tube. Condensation of sulfur on the quartz window was avoided by constant heating of the window with a small gas flame.

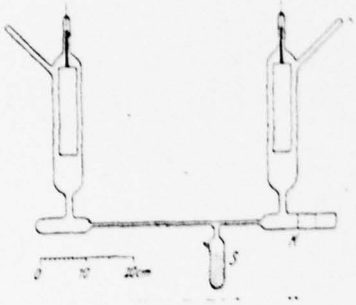


Figure 1: S_2 light source

The discharge through the tube was powered by a 5 kVA transformer at 12,000 V. The sulfur in S was heated to about 170° C by an electric oven, and the discharge tube was evacuated with an oil diffusion pump. The transformer was turned on only intermittently. When the vacuum in the discharge tube was high enough to sustain a discharge, there was a very powerful S_2 light source which could be photographed through the quartz window.

The light from this source passed through a slit and fell on a 6.4 m grid manufactured with the aid of the machine of Prof. Gale in Chicago, and installed in a Paschen mount. The mounting is described in greater detail in the previously cited work of this author [5].

The (1.14), (2.17) and (3.17) bands were photographed on Eastman-Kodak No. 33 plates, while the other bands were recorded on Eastman-Kodak No. IIIF plates. The plates were 2"x18" and about 1 mm thick. With the No. 33 plates, a half-minute exposure of the iron arc spectrum as reference spectrum was sufficient, but with the IIIF plates the exposure of the reference spectrum had to be extended to one minute. In the region above 5800 Å, neon was also used as a reference spectrum. It was possible for the neon to be introduced to the discharge tube before the sulfur

was heated. When the transformer was turned on, there was then an intense neon light source. Exposures of the reference spectra were made before each exposure of the sulfur spectrum, with the upper half of the plate covered. Immediately after the reference exposures were made, the cover was removed. For photographs of the (1.14), (2.17) and (3.17) bands, a Corning-Noviol filter No. 3389 absorbing all light below about 4210 Å was placed before the slit, and for photographs of the other bands, a Noviol filter No. 3385 absorbing light below about 4800 Å was used. About two hours was sufficient time for the exposure of the (1.14) band with its head at 4433.6 Å, (2.17) at 4747.6 Å and (3.17) at 4051.3 Å at the third order of the grid with a current of 18 amperes in the primary winding of the transformer. Exposures of the (3.19) band with its head at 4937.2 Å, (4.19) at 4842.2 Å, (4.22) at 5309.9 Å, (5.22) at 5193.7 Å, (5.23) at 5359.7 Å, (6.23) at 5249.8 Å, (6.25) at 5596.1 Å, (7.25) at 5472.5 Å, (7.27) at 5840.2 Å and (8.27) at 5709.6 Å, on the other hand, required about 20 hours at the third order. Although the grid chamber was held at a constant temperature with a toluol regulator and a heating coil on a movable ventilator, the briefer exposures were sharper.

The plates were evaluated on an Abbé-type comparator built by K. Gürgen in the workshop of the Institute. The 20 cm long calibrated glass scale and the spiral type measuring microscope were obtained from C. Zeiss, Jena. With this microscope it was possible to measure the sharp lines to a precision of 0.001 mm. In the fourth order, where the dispersion of the grid was about 0.57 Å per mm, the wavelengths of the lines could thus be determined to a precision of 0.001 Å. This would mean a precision of about 0.003 cm^{-1} for the wave numbers. However, since with the large dispersion a number of lines were double or fuzzy, a precision of only 0.01 cm^{-1} has been relied upon.

The wavelengths of the reference spectra were drawn from the "M.I.T. Wavelength Tables (1939)" compiled by Harrison.

The wave numbers of the spectral lines were calculated according to the following method: for the measurement of each band, three measurement lines were chosen, one of which lay about in the middle of the band to be measured, and the other two of which lay at the two ends of the band. A second degree equation for the wavelengths was calculated from these three lines. The precision of this equation was checked by comparison of the computed wavelengths of the intermediate Fe or Ne lines with the wavelengths given in Harrison's tables. If the agreement was satisfactory (within 0.003 Å), the equation was used to compute the wavelengths of points on the plate lying 1 mm apart. These wavelengths were converted to wave numbers in a vacuum using Kayser's "Wave Number Table." The scattering was then known as a wave number for each millimeter of the plate, and the wave numbers of the lines lying in any millimeter-region were computed by interpolation using a Marchant model CT10M computer.

The resolution in the fourth order of the grid was about 300,000, which is about 75 percent of the value to be expected from a grid with a surface of 5.5 inches and 18,000 lines per inch. Even with this high resolution, a few lines were not resolved.

III. Results

The S_2 bands are cut off toward the red. Under higher dispersion, the undistorted bands appear to have a strong and a weak peak, the latter lying about 7 or 8 cm^{-1} to the violet side of the former. In the distorted bands (2.16) and (2.17), the weaker peak appears to lie about 31 cm^{-1} to the violet side of the strong peak, at (4.19), (4.22), (6.23), (6.24) and (6.25) about 27 cm^{-1}, and at (7.25) and (7.27) about 25 cm^{-1} to the short wave side of the stronger peak. The strong peaks are clearest at lower dispersions, and generally were measured as the band head and used in the vibrational analysis.

Almost all lines of the (3.17), (3.19), (5.22) and (5.23)

bands could be divided into six spectral branches. It was also possible to find six spectral branches in the (2.16), (4.19) and (4.22) bands, but in the other bands it was possible to find only four branches. The other two are probably too weak, but it is noteworthy that not all the band lines could be classified in the four branches found.

The six branches agree with the three R and three P branches one would expect from a $^3\Sigma - ^3\Sigma$ transition. The results agree with the analysis of Olsson [5] and are also analogous to the analysis of the Schumann-Runge bands of O_2 which were analyzed by Ossenbrüggen [6] and by Lochte-Holtgreven and Dieke [7].

Tables 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13 and 14 give the wave numbers of the branches of the (1.14), (2.17), (3.17), (3.19), (4.19), (4.22), (5.22), (5.23), (6.23), (6.25), (7.25), (7.27) and (8.27) bands. The classification of the branches as R_1, R_2, R_3, P_1, P_2 and P_3 branches will be discussed below. In the first column is found the quantum number K of the lines of the branch. Then follows the wave number of the line in cm^{-1}. The number in parentheses after each wave number indicates a visual estimation of the line intensity on the photographic plate. f or d after this number indicates respectively a blurred or double line. The number outside the parenthesis indicates the number of lines associated with the band, if it is more than one. The lines of the R_1 and P_1 branches of the (2.17) band could not be pursued down to the small K numbers. This is probably to be ascribed to the distortions described above.

Table 2: Wave numbers of lines of the (1.14) band

K	R_1	R_2	R_3	P_1	P_2	P_3
1	22556,14 ($\frac{1}{2}$)^2	—	—	22553,94 (1)^2	—	—
3	56,14 ($\frac{1}{2}$)^2	—	—	52,37 (2)^2	—	—
5	55,83 ($\frac{1}{2}$)	22548,44 (2f)^2	22548,96 (0)	50,37 (2)^2	22543,57 (0)	22544,43 (1)
7	55,05 ($\frac{1}{2}$f)	47,96 (3)^3	48,44 (2f)^2	47,96 (3)^3	41,36 ($\frac{1}{2}$)	42,30 (1)
9	53,94 (1)^2	47,13 (2)	47,62 (0)	45,13 (5)^2	38,70 ($\frac{1}{2}$)	39,81 ($\frac{1}{2}$)
11	52,37 (2)^2	45,80 (2)	46,43 (1)	41,93 (4)^2	35,63 ($\frac{1}{2}$f)	36,84 ($\frac{1}{2}$)
13	50,37 (2)^2	44,12 (2)	44,80 (1)	38,21 (3)^2	32,21 ($\frac{1}{2}$)	33,40 (2)
15	47,96 (3)^3	42,02 (1)	42,69 (2)	34,10 (4)^2	28,35 (1)	29,54(10f)^5
17	45,13 (5)^2	39,51 (1)	40,21 (2)	29,54(10f)^5	24,05 (1)	25,29 (4)^2
19	41,93 (4)^2	36,58 (2)	37,15 (1)	24,61 (6)^2	19,31 (2)	20,43 (2)
21	38,21 (3)^2	33,25 (2)	33,62 (2)	19,22 (4)^2	14,27 (4)^2	15,21 (1)
23	34,10 (4)^2	29,54(10f)^5	29,54(10f)^5	13,38(2d)^2	08,75 (2)	09,48 (1)
25	29,54(10f)^5	25,29 (4)^2	25,07 (2)	07,17 (2)	02,82 (1)	03,21 ($\frac{1}{2}$d)
27	24,61 (6)^2	20,75 (2)	19,93 (2)	00,49 (2)	22496,48 (4)^2	22496,48 (4)^2
29	19,22 (4)^2	15,78 (3)	14,27 (4)^2	22493,40 (2)	89,75 (3)	89,20 (1f)
31	13,38(2d)^2	10,38 (4)	08,01 (1)	85,85 (1)	82,58 (4)	81,35 (1)
33	06,96 (2)	04,54 (2)	01,08 (2)	77,78 (2)	75,02 (1)	72,87 (1)
35	00,19 (1)	22498,28 (1)	22493,51 (2)	69,33 (2)	67,04 (3)	63,81 (1)
37	22492,76 (4)	91,55 (3)	85,28 ($\frac{1}{2}$f)	60,31 (4)	58,61 (2)	54,03 (2)
39	84,94 (1)	84,23 (2)	76,40 (1)	50,83 (2)	49,72 (4)	43,62 ($\frac{1}{2}$)
41	76,60 (1)	—	66,79 (1)	40,84 (1)	40,23 (2)	32,47 ($\frac{1}{2}$)
43	67,60 (1)	—	56,57 ($\frac{1}{2}$f)	30,30 (1)^2	30,30 (1)^2	—
45	58,04 (1)	—	—	19,20 (1)	—	—
47	47,84 (1)	—	—	07,48 (1)	—	—
49	37,01 ($\frac{1}{2}$)	—	—	22395,16 (1)	—	—
51	25,45 (2)	—	—	82,16 ($\frac{1}{2}$)	—	—
53	13,33 ($\frac{1}{2}$f)	—	—	68,50 (1)	—	—
—	—	—	—	54,13 ($\frac{1}{2}$)	—	—
—	—	—	—	39,19 (0)	—	—

Table 3: Wave numbers of lines of the (2.17) band

K	R_1	R_2	R_3	P_1	P_2	P_3
17	—	—	21060,33 (2)	—	—	21045,23 (0)
19	—	21046,98 (1)	57,85 (1)	—	21029,94 (3)	40,96 (3)
21	—	44,29 (3)	54,96 (2)	—	25,16 (1)	36,36 (1f)
23	—	40,51 (3)	51,69 (2f)	—	20,18 (4)^2	31,30 (1f)
25	—	36,50 (4f)	47,89 (3)	—	14,35 (2)	25,77 (1)
27	—	32,10 (2)	43,73 (2)	—	08,16 (2)	19,87 ($\frac{1}{2}$)
29	—	27,35 (3)	39,10 (3)	—	01,66 (4)	13,56 (4)
31	21045,05 (2)	22,26 (2)	34,08 (3)	21017,75 (1)	20994,79 (4)	06,79 (2)
33	39,33 (3)	16,78 (4)	28,62 (3)	10,16 (2)	87,56 (3)	20999,60 (2)
35	33,27 (6)	10,84 (5)	22,71 (2)	02,32 (2)	79,92 (2)	91,97 (1)
37	26,88 (5)	04,49 (4)	16,30 (3)	20994,15 (7)^2	71,84 (6f)^2	83,90 (2)
39	20,18 (4)^2	20997,74 (10)^2	09,42 (2)	85,67 (5)^2	63,44 (2)	75,36 (3)
41	13,05 (4)	90,56 (4)	02,04 (3)	76,82 (2)	54,54 (3)	66,32 (5f)^2
43	05,59 (3)	82,94 (3)	20994,15 (7)^2	67,58 (3)	45,26 (3f)^2	56,86 (2)
45	20997,74 (10)^2	74,84 (2)	85,67 (5)^2	58,01 (3)	35,48 (3)	46,82 (2)
47	89,47 (3)	66,32 (5f)^2	76,61 (1)	48,03 (3)	25,29 (2)	36,22 (1)
49	80,82 (2f)	57,20 (2)	66,85 (2)	37,69 (4)	14,59 (2)	25,02 (2)
51	71,84 (6f)^2	47,56 (4)	56,38 (1)	26,97 (3)	03,38 (2)	13,16 (1)
53	62,33 (2)	37,34 (2)	45,26 (3f)^2	15,78 (4)	20891,65 (3)	00,54 (1)
55	52,45 (3f)	26,54 (2f)	—	04,23 (3)	79,33 (3)	20887,14 ($\frac{1}{2}$)
57	42,13 (2)	14,95 (1)	—	20892,24 (3)	66,37 ($\frac{1}{2}$)	73,12 (1)
59	31,32 (2)	02,69 (1)	—	79,83 (3)	52,76 ($\frac{1}{2}$f)	—
61	19,94 (2f)	20889,60 ($\frac{1}{2}$)	—	66,90 (2)	38,39 (2)	—
63	07,93 (1)	75,64 (1)	—	53,40 (5)^2	23,14 (0)	—
65	20895,48 (1)	—	—	39,51 (1)	—	—
67	82,20 (2)	—	—	24,62 (0)	—	—
69	68,30 (1f)	—	—	—	—	—

Table 4: Wave numbers of lines of the (3.17) band

K	R_1	R_2	R_3	P_1	P_2	P_3
3	21497,71 (0)	—	21491,19 (2)[3]	21493,93 (0)	—	21488,89 (3f)[2]
5	21497,51 ($\frac{1}{2}$)	21491,19 (2)[3]	21491,19 (2)[3]	21492,13 (2f)	—	87,11 (2)[3]
7	96,88 (1)	90,53 (1)	90,86 (2)	89,78 (3)	—	85,04 (1f)
9	95,85 (2)	89,51 (1)	90,18 (4f)[3]	87,11 (2)[3]	21481,38 (2)	82,48 (2f)[2]
11	94,36 (2)	88,07 (1)	88,59 (3f)[2]	83,96 (2)[2]	78,26 (2f)	79,51 (2)[2]
13	92,52 (2)	86,20 (2)	87,11 (2)[3]	80,47 (2)	74,66 (0f)	75,96 (1)
15	90,18 (4f)[3]	83,96 (2)[2]	85,04 (1f)	76,52 (2)	70,65 (2)[2]	72,21 (6)[3]
17	87,57 (2)	81,23 (3)	82,48 (2f)[2]	72,21 (6)[3]	66,28 (4)[2]	67,90 (6)[2]
19	84,49 (2)	78,10 (1f)	79,51 (2)[2]	67,39 (2)	61,47 (6f)[2]	63,13 (1)
21	80,96 (3)	74,58 (1f)	76,10 (4)	62,21 (3)	56,25 (4f)	57,96 (2)
23	76,99 (1)	70,65 (2)[2]	72,21 (6)[3]	56,60 (3)	50,56 (4)[2]	52,41 (3)
25	72,65 (2)	66,28 (4)[2]	67,99 (2)	50,56 (4)[2]	44,47 (2)	46,41 (3)
27	67,90 (6)[2]	61,55 (6f)[2]	63,34 (2)	44,11 (3)	37,96 (2)	40,03 (3)[2]
29	62,72 (4)	56,44 (3)	58,23 (3)	37,23 (2)	31,14 (2)	33,16 (3)
31	57,08 (4)	50,95 (5f)	52,62 (2)	29,92 (3)	23,88 (2)	25,90 (4)
33	51,08 (5f)	45,02 (4f)	46,57 (3f)	22,19 (2)	16,24 (1)	18,16 (3f)
35	44,58 (2)	38,74 (1)	40,03 (3)[2]	14,05 (2)	08,27 (2f)[2]	09,95 (3)
37	37,69 (2)	32,07 (2)	33,02 (3)	05,48 (4)	21399,84 (1f)	01,27 (3)
39	30,37 (5)	25,00 (3)	25,41 (4)	21396,47 (4)[2]	90,99 (2)	21392,11 (2)
41	22,60 (2)	17,56 (2)	17,14 (1f)	87,06 (4)	81,80 (2)	82,32 (3)
43	14,38 (3)	09,71 (3)	08,27 (2f)[2]	77,17 (3)	72,16 (4f)	72,02 (2f)
45	05,68 (2f)	01,46 (2)	21398,73 (2)	66,82 (3f)	62,30 (2)	61,00 (3f)
47	21396,47 (4)[2]	21392,81 (3)	88,27 (1)	55,98 (3)	51,94 (3)	49,25 (1)
49	86,72 (2)	83,65 (4)	77,06 ($\frac{1}{2}$)	44,69 (2)	41,15 (2)	36,71 ($\frac{1}{2}$)
51	76,38 (2)	74,05 (2)	65,18 ($\frac{1}{2}$)	32,85 (3)	29,89 (2)	23,46 (2)
53	65,44 (1)	63,95 (2)	—	20,41 (3)	18,02 (2)	09,53 (0f)
55	53,78 (2)	53,55 (2)	—	07,34 (1)	05,82 (2)	—
57	41,37 (0)	42,77 (1)	—	21293,59 (1)	—	—
59	28,12 ($\frac{1}{2}$)	—	—	79,07 ($\frac{1}{2}$)	—	—
61	13,93 (0)	—	—	63,69 (2)	—	—
—	—	—	—	47,41 (1)	—	—

Table 5: Wave numbers of lines of the (3.19) band

K	R_1	R_2	R_3	P_1	P_2	P_3
5	20257,10 (0)	—	—	20251,67 (0)	—	—
7	56,38 (0)	20249,19 (1d)	—	49,26 (1)	—	—
9	55,47 ($\frac{1}{2}$)	48,56 (1)	—	46,72 (1)	20240,40 (2)[2]	—
11	54,18 (1)	47,25 (1)	20247,95 (3f)	43,76 (1)	37,48 ($\frac{1}{2}$)	—
13	52,45 (1)	45,57 ($\frac{1}{2}$)	46,48 (0)	40,40 (2)[2]	34,05 (2)[2]	20235,37 (0)
15	50,37 (1)	43,51 (1)	44,59 (1)	36,68 (1)	30,26 (1)	31,71 ($\frac{1}{2}$)
17	47,90 (3)	40,99 (1)	42,24 (1)	32,48 (1)	26,06 (1)	27,63 (2)
19	45,02 (2)	38,11 (3)[2]	39,53 (1)	27,94 (2)	21,45 (1)	23,17 (3)
21	41,75 (2)	34,83 (1)	36,34 (2)	23,03 (3)	16,46 (1f)	18,26 (1)
23	38,11 (3)[2]	31,19 (1)	32,88 (1)	17,69 (1)	11,08 (1f)	13,06 (4)[2]
25	34,05 (2)[2]	27,16 (2)	28,92 (3)	11,95 (2)	05,33 (1)	07,32 (4)[2]
27	29,61 (2)	22,80 (2)	24,62 (2)	05,83 (2)	20199,25 (5)[2]	01,25 (2)
29	24,78 (3)	18,05 (2)	19,87 (2)	20199,25 (5)[2]	92,71 (1)	20194,83 (3f)
31	19,55 (2)	12,96 (4)[2]	14,66 (2f)	92,37 (3)	85,87 (2)	87,89 (1)
33	13,94 (2)	07,40 (4)[2]	09,05 (2)	85,07 (3)	78,63 (4)	80,60 (3f)
35	07,92 (3)	01,56 (4f)[2]	02,99 (2)	77,37 (2)	71,05 (3)	72,86 (2)
37	01,46 (4f)[2]	20195,39 (3)	20196,41 (2)	69,26 (1)	63,13 (3)	64,69 (2)
39	20194,65 (3f)[2]	88,52 (3f)	89,31 (3)	60,74 (2)	54,80 (2)	56,00 (2)
41	87,40 (2)	81,91 (3)	81,65 (2)	51,83 (2)	46,12 (2)	46,75 (1)
43	79,72 (3f)	74,63 (2)	73,29 (2)	42,49 (2)	37,09 (3f)	36,98 (2f)
45	71,55 (2)	66,97 (3)	64,26 (1)	32,72 (1f)	27,72 (3)	26,58 (1)
47	62,98 (2)	58,89 (2)	54,46 (0)	22,49 (3)	17,97 (2)	15,39 ($\frac{1}{2}$)
49	53,86 (1)	50,38 (3)	43,81 (0)	11,77 (2)	07,80 (1)	03,50 (0)
51	44,17 (1)	41,25 (1)	—	00,59 (1)	20097,23 (1)	—
53	33,81 (1f)	—	—	20088,78 (2)	86,02 (2)	—
55	22,93 ($\frac{1}{2}$)	—	—	76,46 (1)	—	—
57	11,20 ($\frac{1}{2}$)	—	—	63,43 (0)	—	—
59	20098,72 (0)	—	—	49,69 ($\frac{1}{2}$)	—	—

Table 6: Wave numbers of lines of the (4.19) band

K	R_1	R_2	R_3	P_1	P_2	P_3
7	20673,48 ($\frac{1}{2}$)	20646,94 ($\frac{1}{2}$f)	—	—	20640,52 ($\frac{1}{2}$)	—
9	71,98 (1f)	45,92 ($\frac{1}{2}$)	—	20663,11 ($\frac{1}{2}$)	37,80 (2)	—
11	70,32 (5)	44,66 (2)	20656,39 ($\frac{1}{2}$)	60,23 ($\frac{1}{2}$f)	34,78 (1)	20646,94 ($\frac{1}{2}$)
13	68,40 (3)	43,14 ($\frac{1}{2}$)	55,02 ($\frac{1}{2}$)	—	31,56 (4)	43,76 (0)
15	66,00 ($\frac{1}{2}$)	41,19 (2)	53,18 (1)[2]	52,69 (3)	27,86 (1)	40,17 ($\frac{1}{2}$)
17	63,38 ($\frac{1}{2}$)	38,87 (2)	50,94 (1)	48,14 ($\frac{1}{2}$)	23,78 (6)[2]	36,14 (5)[2]
19	60,35 (1)	36,14 (5)[2]	48,33 ($\frac{1}{2}$)	43,43 (0)	19,51 (2)	31,86 (0)
21	56,97 (2)	33,04 (3)	45,30 (1)	38,41 ($\frac{1}{2}$)	14,53 (2)	27,04 (5)[2]
23	53,18 (1)[2]	29,44 (4)	41,83 (1f)	32,92 (2)	09,24 (4)	21,86 (2)
25	49,04 (1)	25,50 (2)	37,81 (2)	27,04 (3)[2]	03,63 (3)[2]	16,34 ($\frac{1}{2}$)
27	44,49 (1)	21,15 (4)	33,40 ($\frac{1}{2}$)[2]	20,84 (1)	20597,56 (2f)	10,15 ($\frac{1}{2}$)
29	39,55 (4)	16,44 (d)[2]	28,55 (2)[2]	14,13 (1)	91,11 (2)	03,63 (3)[2]
31	34,21 (3)	11,17 (2f)	23,27 (0)	07,18 (2d)	84,26 (5)	20596,57 ($\frac{1}{2}$)
33	28,55 (2)[2]	05,36 (2)	17,40 (0)	20599,73 (4)	76,87 (3)	89,16 (0)
35	22,44 (1)	20599,18 (2)	11,11 (1f)	91,98 (2)	68,96 (1)	—
37	15,85 (1f)	91,98 (2)	—	83,79 (3)	60,75 (3f)	—
39	08,88 (2)	85,76 (2)	—	75,14 (3f)	51,41 ($\frac{1}{2}$)	—
41	01,50 (2)	78,16 (1)	—	66,09 (2)	43,10 (1)	—
43	20593,67 (2)	70,16 (3)	—	56,67 (3)	34,33 ($\frac{1}{2}$)	—
45	85,15 (0)	—	—	46,72 (1)	—	—
47	76,12 (0)	—	—	36,08 (4f)	—	—
49	66,62 ($\frac{1}{2}$)	—	—	25,03 (2)	—	—
51	56,33 (4)	—	—	13,28 (0)	—	—
53	45,62 ($\frac{1}{2}$)	—	—	—	—	—
55	34,33 ($\frac{1}{2}$)	—	—	20488,37 (0)	—	—

Table 7: Wave numbers of lines of the (4.22) band

K	R_1	R_2	R_3	P_1	P_2	P_3
3	18855,68 (0)	—	—	—	—	—
5	55,36 (0)	18828,03 (2)	—	—	—	—
7	54,83 (0)	27,76 (1)	—	—	—	—
9	53,82 ($\frac{1}{2}$)	27,11 (0f)	—	18845,28 (3)	18818,81 (3f)[2]	—
11	52,46 ($\frac{1}{2}$f)	26,14 (2)	18837,71 ($\frac{1}{2}$f)	42,32 (1)	16,23 ($\frac{1}{2}$f)	—
13	50,86 (3)	24,89 (1)	36,73 ($\frac{1}{2}$)	39,06(1fd)	13,26 (1)[2]	18825,43 (3f)[2]
15	48,94 (2f)	23,20 (3)	35,19 (1)	35,36 (2f)	09,86 (2f)	22,21 (1f)[2]
17	46,57 (1)	21,17 (5f)	33,31 ($\frac{1}{2}$)	31,41 ($\frac{1}{2}$)	06,07 (4fd)	18,59 ($\frac{1}{2}$f)
19	43,95 (2)	18,81 (3f)[2]	31,03 ($\frac{1}{2}$)	27,03 (0f)	02,05 (1)	14,57 (1f)
21	40,89 (2)	16,09 (2f)	28,39 ($\frac{1}{2}$)	22,27 (1f)	18797,53 (2f)	10,14 (4f)[2]
23	37,56 (2f)	13,00 (2)	25,43 (3f)[2]	17,28 (2)	92,76 (2)	05,50 (2)
25	33,91 (2)	09,50 (2)	21,83 (2)	11,88 (3)	87,61 (2)	00,31 ($\frac{1}{2}$)
27	29,84 (5)	05,64 (3)	17,74 (2f)	06,16 (4d)	82,07 (3)	18794,62 (2f)
29	25,43 (3f)[2]	01,42 (2)	13,26 (1)[2]	00,05 (1)	76,19 (3)	88,43 ($\frac{1}{2}$f)
31	20,68 (3)	18796,82 (2)	08,37 (1)	18793,65 (1)	69,90 (3)	—
33	15,64 (3f)	91,65 (2)	—	86,89 (2)	63,16 (3)	—
35	10,14 (4f)	—	—	79,70 (3)	55,94 (4f)[2]	—
37	04,34 (4f)	—	—	72,26 (2)	—	—
39	18798,10 (2)	—	—	64,37 (3)	—	—
41	—	—	—	56,00 (3)	—	—
43	—	—	—	47,16 (2)	—	—
45	—	—	—	—	—	—

Table 8: Wave numbers of lines of the (5.22) band

K	R_1	R_2	R_3	P_1	P_2	P_3
5	19257,57 (0)	19248,15 (1f)^2	19248,15 (1f)^2	19252,24 (0)	—	—
7	56,84 (0)	—	19247,96 (2f)^2	50,04 (1f)	19241,21 (0)	19242,18 (0)
9	55,80 (0)	46,60 (0)	47,24 ($\frac{1}{2}$f)	—	38,65 ($\frac{1}{2}$)	39,78 (0)
11	54,41 (1f)	45,31 ($\frac{1}{2}$)	46,10 ($\frac{1}{2}$)	44,29 (0)	35,73 (0)	36,98 ($\frac{1}{2}$)
13	52,67 ($\frac{1}{2}$)	43,62 ($\frac{1}{2}$)	44,64 ($\frac{1}{2}$)	40,92 ($\frac{1}{2}$)	32,33 (0)	33,78 (1)
15	50,51 ($\frac{1}{2}$)	41,63 (1f)	42,78 ($\frac{1}{2}$)	37,10 (2f)	28,60 ($\frac{1}{2}$)	30,17 (0)
17	47,96 (2f)^2	39,18 ($\frac{1}{2}$)	40,51 (2)	32,98 (1)	24,48 (4)^2	26,22 (1f)
19	45,04 (1)	36,38 ($\frac{1}{2}$f)	37,85 (2)	28,40 (1)	19,99 (1)	21,76 ($\frac{1}{2}$)
21	41,74 (1f)	33,20 (3)	34,77 (2)	23,42 (2)	15,13 ($\frac{1}{2}$)	16,99 (5)^2
23	38,02 (1)	29,69 (1)	31,27 (2)	18,08 (5f)^2	09,89 ($\frac{1}{2}$)	11,83 (1)
25	33,91 (1)	25,78 (2f)	27,37 (2f)	12,30 (3)	04,31 (1)	06,21 (8)^2
27	29,40 (1)	21,55 (2)	22,98 (1)	06,21 (8)^2	19198,36 ($\frac{1}{2}$)	00,21 ($\frac{1}{2}$f)
29	24,48 (4)^2	16,99 (5)^2	18,16 (5f)^2	19192,63 (1f)	92,06 (2)	19193,77 (2)
31	19,16 (2)	12,01 (2)	12,83 (2)	92,69 (3)	85,36 (5f)^2	86,86 (2)
33	13,38 (1)	06,72 (2)	06,96 (1)	85,36 (5f)^2	78,40 (2)	79,42 (1)
35	07,19 ($\frac{1}{2}$)	01,05 (2)	00,49 (4)^2	77,51 (2)	70,98 (1)	71,49 (1)
37	00,49 (4)	19195,03 (2f)	93,32 (4)^2	69,19 (2f)	63,31 (2)	62,89 ($\frac{1}{2}$)
39	19193,32 (4)^2	88,58 (2)	85,46 (3f)^2	60,53 (3)	55,17 (2)	53,69 ($\frac{1}{2}$)
41	85,46 (3f)^2	81,56 (2f)	76,73 ($\frac{1}{2}$)	51,25 ($\frac{1}{2}$)	46,67 (1)	43,63 ($\frac{1}{2}$)
43	77,15 (0)	73,46 ($\frac{1}{2}$)	67,30 (0)	41,49 (1)	37,63 (1)	—
45	68,13 ($\frac{1}{2}$)	—	57,03 (0f)	31,07 (1)	27,44 ($\frac{1}{2}$)	21,38 (0)
47	58,32 (0)	—	46,16 (0)	19,95 ($\frac{1}{2}$)	—	09,06 (0)
49	47,58 (0)	—	—	08,06 ($\frac{1}{2}$)	—	19096,17 (0f)
51	36,06 (0)	—	—	19095,37 (1)	—	—
—	—	—	—	81,76 (2)	—	—

Table 9: Wave numbers of lines of the (5.23) band

K	R_1	R_2	R_3	P_1	P_2	P_3
5	18662,77 (0f)	18652,89 (6f)	—	57,52 (0)	18648,36 (0)	—
7	62,20 (2)	—	—	55,41 (1)	46,30 (0)	—
9	61,28 (1)	51,74 ($\frac{1}{2}$f)	18652,33 (0f)	52,89 (6f)	43,78 (0)	—
11	59,99 (2)	50,52 (1)	51,29 ($\frac{1}{2}$)	49,90 (3f)	40,90 ($\frac{1}{2}$)	18642,16 (0f)
13	58,31 (1)	48,91 (2)	49,90 (3f)	46,55 (1)	37,63 (1)	39,01 (3)
15	56,24 (3)	46,98 (1)	48,20 ($\frac{1}{2}$)	42,86 (1)	33,99 (1)	35,57 (5)
17	53,81 (2)	44,69 (2)	46,01 (2)	38,79 (2)	29,97 (3fd)	31,69 (1)
19	51,01 (2)	42,04 (2f)	43,47 (1)	34,35 (2)	25,61 (2)	27,42 (1)
21	47,81 (2)	39,01 (3)	40,56 (4)	29,50 (2)	20,90 (2)	22,79 (1)
23	44,24 (3)	35,57 (5)	37,20 (2)	24,29 (3)	15,81 (2)	17,74 (2)
25	40,32 (3)	31,86 (3)	33,44 (2)	18,67 (5)	10,37 (2)	12,35 (3)
27	35,96 (2)	27,81 (3)	29,26 (3)	12,74 (2)	04,59 (2)	06,41 (5)
29	31,22 (2)	23,40 (4)	24,62 (2)	06,41 (5)	18598,47 (2)	00,21 (1)
31	26,09 (3)	18,67 (5)	19,51 (2)	18599,60 (3)	91,99 (4)	18593,56 (3fd)
33	20,53 (2)	13,55 (3)	13,85 (2)	92,44 (2)	85,21 (3)	86,36 (5fd)
35	14,55 (4)	08,10 (6)	07,58 (2)	84,85 (3)	78,07 (3)	78,57 (2)
37	08,10 (6)	02,31 (3)	00,67 (1)	76,81 (4)	70,60 (2)	70,26 (1)
39	01,13 (2)	18596,14 (3)	18593,03 (1)	68,36 (2)	62,75 (2)	61,27 (1)
41	18593,63 (3fd)	89,42 (2)	84,65 (2)	59,37 (3)	54,51 (3)	51,55 (2f)
43	85,56 (2)	81,57 (2)	75,41 ($\frac{1}{2}$)	49,85 (1)	45,73 (3)	40,99 (4f)
45	76,81 (4)	—	65,47 ($\frac{1}{2}$)	39,73 (1)	35,83 (1)	29,78 (2)
47	67,27 ($\frac{1}{2}$)	—	54,97 (2)	28,93 (1)	—	17,88 ($\frac{1}{2}$)
49	56,88 (2f)	—	—	17,36 ($\frac{1}{2}$)	—	—
51	45,73 (3)	—	—	05,02 ($\frac{1}{2}$)	—	—
53	—	—	—	18491,76 ($\frac{1}{2}$)	—	—
55	20,41 ($\frac{1}{2}$)	—	—	77,57 (0)	—	—

Table 10: Wave numbers of lines of the (6.23) band

K	R_1	R_2	P_1	P_2
5	—	19039,08 (1)	—	—
7	19065,76 ($\frac{1}{2}$)	38,57 (3)	—	19032,34 ($\frac{1}{2}$)
9	64,57 (0)	37,83 (6)[2]	19056,32 (1)[2]	29,86 (1)
11	63,02 (1f)	36,66 (3)	53,13 (3)	27,00 (1)
13	61,16 (2f)	35,03 (6)	49,66 ($\frac{1}{2}$)	23,69 (2)
15	58,86 (3f)	33,12 (8)[2]	45,64 (2)	20,13 (2)
17	56,32 (1)[2]	30,76 (3)	41,41 (2)	16,09 (3)
19	53,38 (2)	27,96 (6)	36,79 (2f)	11,71 (4)
21	50,04 (2)	24,73 (3)	31,89 (1)	06,83 (2)
23	46,35 (3)	21,11 (3)	26,58 (2)	01,57 (10f)[3]
25	42,31 (2)	16,99 (2)	20,76 (2)	18995,91 (5)
27	37,87 (6)[2]	12,43 (6f)	14,77 (2)	89,75 (4)
29	33,12 (8)[2]	07,27 (4f)	08,38 (2)	83,08 (3)
31	27,85 (2)	01,57 (10f)[3]	01,49 (2f)	75,90 (3)
33	22,14 (6f)	18995,27 (3)	18994,21 (4)	68,19 (2)
35	15,89 (2)	88,26 (2)	84,43 (5)	59,82 (3)[2]
37	09,11 (1f)	80,52 (4)	78,17 (5)	50,78 (3)
39	01,60 (10f)[3]	71,84 (1)	69,36 (1)	40,90 (3f)
41	18993,43 (3)	62,26 (3)	59,82 (3)[2]	30,22 (1)
43	84,24 (3)	51,68 (2)	49,63 (1)	18,64 (2)
45	75,60 (5)	40,07 (3)	38,41 ($\frac{1}{2}$)	06,01 ($\frac{1}{2}$)
47	64,87 (0)	27,56 (1)	27,07 (0)	18892,38 (1)
49	—	13,96 (2)	14,91 (1)	77,67 ($\frac{1}{2}$f)
51	—	18899,28 (3)	—	62,18 (1)

Table 11: Wave numbers of lines of the (6.25) band

K	R_1	R_2	P_1	P_2
	—	17866,43 (0)	—	17861,89 ($\frac{1}{2}$f)
7	17894,05 (0)	66,11 (1)[2]	17887,06 (0)	59,86 (0f)
9	92,96 ($\frac{1}{2}$)	65,40 ($\frac{1}{2}$)	84,44 ($\frac{1}{2}$)	57,48 (2)
11	91,52 (1)	64,41 (3f)	81,49 (0f)	54,74 ($\frac{1}{2}$)
13	89,76 (1f)	62,98 (3)	78,18 (0)	51,68 (1)
15	87,71 (0)	61,24 (3)	74,51 ($\frac{1}{2}$)	48,28 (2)
17	85,29 (3)	59,04 (3)[2]	70,48 (1)	44,43 (1)
19	82,56 (1f)	56,51 (2)	66,11 (1)[2]	40,24 (3)
21	79,55 (2)	53,59 (2f)	61,37 (3)	35,66 (3)
23	76,21 (3f)	50,23 (1f)	56,36 (2)	30,74 (2)
25	72,42 (3)	46,47 (2)	50,97 (2f)	25,33 (2)
27	68,35 (1)	42,22 (1f)	45,29 (5)	19,52 (2)
29	63,87 (5)	37,47 (8)	39,13 (2)	13,22 (3)
31	59,04 (3)[2]	32,19 (2)	32,66 (4f)	06,47 (2)
33	53,68 (2f)	26,28 (1)	25,78 (2)	17799,17 (1)
35	47,95 ($\frac{1}{2}$)	19,75 (4)	18,45 (6)	91,26 (1)
37	41,65 ($\frac{1}{2}$)	12,43 ($\frac{1}{2}$)	10,71 (2)	82,68 (2f)
39	34,70 ($\frac{1}{2}$)	04,29 (5f)	02,45 (3fd)	73,38 (1)
41	27,00 (6)	17795,26 (0)	17793,49 (2)	63,23 ($\frac{1}{2}$)
43	18,45 (6)	85,26 (0)	83,80 (1)	—
45	—	—	73,38 (1)	—
47	—	—	—	—

Table 12: Wave numbers of lines of the (7.25) band

K	R_1	R_2	P_1	P_2
5	—	18367,87 (3)[s]	—	18363,14 ($\frac{1}{2}$)
7	—	67,62 (2)	—	61,33 (0)
9	—	66,86 (3f)	—	59,00 (3f)
11	—	65,84 (2f)	—	56,19 (1)
13	18391,62 (0f)	64,42 (2)	18380,05 ($\frac{1}{2}$f)	53,13 ($\frac{1}{2}$)
15	89,52 (1)	62,58 (6)	76,43 (0)	49,69 (2)
17	—	60,48 (1f)	72,30 (1f)	45,85 (1)
19	84,15 (0)	58,00 (3f)	67,87 (3)[s]	41,67 (1)
21	80,89 ($\frac{1}{2}$)	55,04 (2)	62,97 (1)	37,13 (4)
23	77,22 (3f)	51,72 (4)	57,68 (1)	32,15 (4)
25	73,28 ($\frac{1}{2}$)	47,95 (4)	52,62 (3)	26,79 (3)
27	68,94 (1)	43,87 (4)	46,09 (1)	21,10 (4)
29	64,21 (2fd)	39,26 (2)	39,73 (3)	14,92 (3)
31	59,14 ($\frac{1}{2}$)	34,03 (2)	33,02 (5)[s]	08,24 (2f)
33	53,58 (1)	27,46 (2f)	25,91 (2)	01,01 (6)
35	47,36 (1)	20,60 (3)	18,32 (3f)	18292,49 (3)
37	40,56 (2)	—	10,13 (1)	83,56 (2fd)
39	33,02 (5)[s]	—	01,44 (1)	—
41	—	—	18292,04 ($\frac{1}{2}$)	—

Table 13: Wave numbers of lines of the (7.27) band

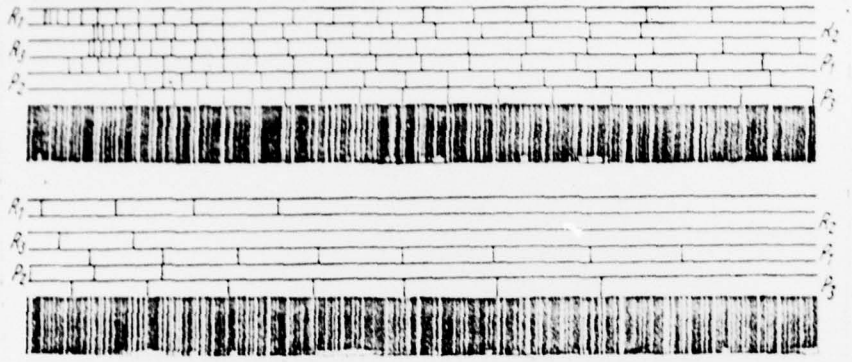
K	R_1	R_2	P_1	P_2
5	—	17118,40 (0)	—	17113,80 (5)[s]
7	—	18,19 (5)	—	11,87 (5)[s]
9	—	17,56 (2)	—	09,57 (10f)[s]
11	17144,75 (5)	16,65 (4)	17134,83 (2f)	06,94 (4f)[s]
13	43,48 (4)	15,38 (8)	31,94 (0)	04,13 (3)
15	41,48 (2)	13,80 (5)[s]	28,35 (2)	00,86 (3)
17	39,19 (1f)	11,87 (5)[s]	24,43 (0)	17097,24 (1)
19	36,56 (2)	09,57 (10f)[s]	20,27 ($\frac{1}{2}$)	93,29 (2)
21	33,61 (3)	06,94 (4f)[s]	15,65 (5)	88,97 (5)
23	30,18 (3f)	03,91 (3)	10,64 (1)	84,34 (3)
25	26,56 (4f)	00,51 (5)	05,34 (4f)	79,33 (2)
27	22,54 (2)	17096,74 (2)	17099,69 (1)	73,95 (4)
29	18,19 (5)[s]	92,50 (3)	93,70 (2)	68,16 (3)
31	13,49 (2)	87,67 (4)	87,40 (3)	61,92 (3)
33	08,37 (3f)	—	80,69 (2)	—
35	02,60 (1)	—	73,59 (3)	—
37	17096,15 ($\frac{1}{2}$)	—	65,86 (6)	—
39	88,97 (5)[s]	—	57,53 (1)	—

Table 14: Wave numbers of lines of the (8.27) band

K	R_2	P_2	K	R_2	P_2
3	17509,28 (1)	17506,62 ($\frac{1}{2}$f)	17	00,25 (2f)	86,04 (3)
5	08,94 (3fd)	04,56 (8)[s]	19	17497,34 (2f)	81,68 (3)
7	08,25 (2f)	02,33 (1)	21	93,18 (1)	76,73 (2)
9	07,29 (3)	17499,65 (1f)	23	89,62 (0)	70,60 (2)
11	06,06 (1f)	96,71 (4)	25	85,08 (0)	63,05 (2)
13	04,56 (8)[s]	93,59 (2f)	27	—	58,54 (0)
15	02,64 (1)	90,03 (2)			

Figure 2 is an extract from the (1.14) band. The six branches making up the band are marked.

Figure 2: The (1.14) band of the S_2 spectrum, with the branches into which the band was analyzed indicated.



The rotation levels of the $^3\Sigma$ states follow the formula

$$F_i = B_v K(K+1)+f_i(K,J-K)+D_v K^2(K+1)^2+\ldots \qquad (1)$$

where B_v and D_v are the rotation constants and J the angular momentum quantum number with the values $J=(K+S),(K+S-1),\ldots,(K-S)$. S is the spin quantum number. For a triplet, S=1, and thus J=(K+1),K,or (K-1). Because of the three values of J, we should have three energy states lying close together for each value of K. These energy states are designated with F_1, F_2, and F_3, ~~corresponding~~ which agree respectively with J=K+1, J=K, and J=K-1. For more details, see Mulliken [8].

Kramers [9] showed that for $^3\Sigma$ states $f_1(K,J-K)$ consists of two parts, one of which is to be ascribed to the interaction of the spin of the electron with the angular momentum, and is given by:

$$\tfrac{1}{2}y[J(J+1)-K(K+1)-S(S+1)] = \tfrac{1}{2}y[J(J+1)-K(K+1)-2] \qquad (2)$$

and the other is to be ascribed to the interaction of the individual electron spins, and is indicated by $w_i K(J-K)$. $f_i(K,J-K)$ therefore becomes

$$f_i K(J-K) = \tfrac{1}{2}y[J(J+1)-K(K+1)-2]+w_i(K,J-K). \qquad (3)$$

Kramers showed further that $w_i(K,J-K)$ has the following values for the three states:

$$\text{for } J=K+1,\ w_1=-\varepsilon[1-3/(2K+3)] \tag{4}$$

$$\text{for } J=K-1,\ w_3=-\varepsilon[1+3/(2K-1)] \tag{5}$$

$$\text{and for } J=K,\ w_2=+2\varepsilon\ . \tag{6}$$

From the combination of equations (3), (4), (5) and (6) is obtained:

$$\text{for } J=K+1,\ f_1=-\varepsilon[1-3/(2K+3)]+yK \tag{7}$$

$$\text{for } J=K-1,\ f_3=-\varepsilon[1-3/(2K-1)]-y(K+1) \tag{8}$$

$$\text{and for } J=K,\ f_2=2\varepsilon-y\ . \tag{9}$$

We now form

$$\Delta_2F_i'(K) = R_i(K)-P_i(K) = F_i'(K+1)-F_i'(K-1)\ . \tag{10}$$

If the f_i are substituted in (1) and the expressions in ε/K are ignored for larger values of K, since ε is usually small, the result is:

$$\text{for } J=K+1,$$
$$\Delta_2F_1'(K) = 2(B_v'+2D_v'+y)+4(B_v'+3D_v')K+12D_v'K^2+8D_v'K^3 \tag{11}$$

$$\text{for } J=K-1,$$
$$\Delta_2F_3'(K) = 2(B_v'+2D_v'-y)+4(B_v'+3D_v')K+12D_v'K^2+8D_v'K^4 \tag{12}$$

$$\text{and for } J=K,$$
$$\Delta_2F_2'(K) = 2(B_v'+2D_v')+4(B_v'+3D_v')K+12D_v'K^2+8D_v'K^3\ . \tag{13}$$

For the lower electron state,

$$\Delta_2F_i''(K) = R_i(K+1)-P_i(K-1) = F_i''(K+1)-F''(K-1) \tag{14}$$

has the same form as (11), (12) and (13). It is only necessary that (') be replaced by (").

In Tables 15a and 15b, the $\Delta_2F_i'(K)$ values are given for v'= 1,2,3 and 4 and for v'=5,6,7 and 8, respectively. In Tables 16a, 16b and in 17a, 17b are given the corresponding $\Delta_1F_2'(K)$ and $\Delta_2F_3'(K)$ values. For v'=1, 2 and 3, the $\Delta_2F_i'(K)$ values are com-

pared with the mean values calculated from Olsson's analysis of the (1.3), (1.4), (2.2), (2.3), (2.4), (3.2) and (3.3) bands. In Tables 18, 19, 20, 21, 22 and 23, the $\Delta_2 F_i''(K)$ values for the vibration levels v"=19, 22, 23, 25 and 27 are compared. The comparisons of the $\Delta_2 F_i'(K)$ and $\Delta_2 F_i''(K)$ values show good agreement and serve as a corroboration of the entire analysis. At the same time the rotational analysis of Olsson and the vibrational analysis of Fowler and Vaidya are confirmed by these results.

The establishment of the R_1 and P_1 branches as R_1, R_2 and R_3 (or P_1, P_2 and P_3) was performed graphically with equations (7), (8) and (9), as in Olsson. Since the results agree with those of Olsson, a description of the method will be omitted.

Table 15a: The $\Delta_2 F_1'(K)$ values of the vibration level with v'=1,2,3,4.

	$\Delta_2 F_1'(K) = F_1'(K+1) - F_1'(K-1) = R_1(K) - P_1(K)$								
	v' = 1		v' = 2		v' = 3		v' = 4		
K	(1,14)	Olsson	(2,17)	Olsson	(3,17)	(3,19)	Olsson	(4,19)	(4,22)
1	2,20	—	—	—	—	—	—	—	—
3	3,77	—	—	—	3,78	—	—	—	—
5	5,44	—	—	—	5,38	5,43	—	—	—
7	7,09	—	—	—	7,10	7,12	—	—	—
9	8,81	—	—	—	8,74	8,75	—	—	8,54
11	10,44	—	—	—	10,40	10,42	—	10,09	10,14
13	12,10	—	—	—	12,05	12,05	—	—	11,80
15	13,86	—	—	—	13,66	13,69	13,76	—	13,58
17	15,59	15,58	—	—	15,36	15,42	15,24	15,24	15,16
19	17,32	17,30	—	—	17,10	17,08	17,02	16,92	16,92
21	18,99	18,98	—	—	18,75	18,72	18,72	18,56	18,62
23	20,72	20,69	—	—	20,39	20,42	20,44	20,26	20,28
25	22,37	22,38	—	22,04	22,09	22,10	22,12	22,00	22,03
27	24,12	24,15	—	23,83	23,79	23,78	23,75	23,65	23,68
29	25,82	25,74	—	25,60	25,49	25,53	25,44	25,42	25,38
31	27,52	27,36	27,30	27,31	27,14	27,18	27,15	27,03	27,03
33	29,18	29,15	29,17	29,21	28,89	28,87	28,88	28,82	28,75
35	30,86	30,67	30,95	30,89	30,53	30,55	30,61	30,46	30,44
37	32,45	32,53	32,73	32,75	32,21	32,20	32,18	32,06	32,08
39	34,11	34,16	34,51	34,45	33,90	33,91	33,87	33,74	33,73
41	35,76	35,72	36,23	36,27	35,56	35,57	35,67	35,41	—
43	37,30	37,30	38,01	37,99	37,21	37,23	—	37,00	—
45	38,84	38,86	39,73	39,75	38,86	38,83	—	38,43	—
47	40,36	40,40	41,44	41,41	40,49	40,49	—	40,04	—
49	41,85	—	43,13	43,14	42,03	42,09	—	41,59	—
51	43,29	—	44,87	44,84	43,53	43,58	—	43,05	—
53	44,83	—	46,55	—	45,03	45,03	—	—	—
55	—	—	48,22	—	46,44	46,47	—	45,96	—
57	—	—	49,89	—	47,78	47,77	—	—	—
59	—	—	51,49	—	49,05	49,03	—	—	—
61	—	—	53,04	—	—	—	—	—	—
63	—	—	54,53	—	—	—	—	—	—
65	—	—	55,97	—	—	—	—	—	—
67	—	—	57,58	—	—	—	—	—	—

Table 15b: The $\Delta_2 F_1'(K)$ values of the vibration level with v'=5,6,7

	$\Delta_2 F_1'(K) = F_1'(K+1) - F_1'(K-1) = R_1(K) - P_1(K)$					
	$v'=5$		$v'=6$		$v'=7$	
K	(5,22)	(5,23)	(6,23)	(6,25)	(7,25)	(7,27)
5	5,33	5,25	—	—	—	—
7	6,80	6,79	—	6,99	—	—
9	—	8,39	8,25	8,52	—	—
11	10,12	10,09	9,89	10,03	—	9,92
13	11,75	11,76	11,60	11,58	11,67	11,54
15	13,41	13,38	13,22	13,20	13,09	13,13
17	14,98	15,02	14,91	14,81	—	14,76
19	16,64	16,66	16,59	16,45	16,28	16,29
21	18,32	18,31	18,15	18,18	17,92	17,96
23	19,94	19,95	19,77	19,85	19,64	19,64
25	21,61	21,65	21,55	21,45	21,26	21,22
27	23,19	23,22	23,10	23,05	22,85	22,85
29	24,85	24,81	24,74	24,74	24,48	24,49
31	26,47	26,49	26,36	26,38	26,12	26,09
33	28,02	28,09	27,93	27,90	27,67	27,68
35	29,68	29,70	29,46	29,50	29,04	29,01
37	31,30	31,29	30,94	30,94	30,43	30,29
39	32,79	32,77	32,24	32,25	31,58	31,41
41	34,21	34,24	33,61	33,51	—	—
43	35,66	35,71	34,57	—	—	—
45	37,06	37,15	35,59	—	—	—
47	38,37	38,34	36,80	—	—	—
49	39,52	39,52	—	—	—	—
51	40,69	40,71	—	—	—	—
53	—	41,75	—	—	—	—
55	—	42,84	—	—	—	—

Table 16a: The $\Delta_2 F_2'(K)$ values of the vibration level with v'=1,2,3,4

	$\Delta_2 F_2'(K) = F_2'(K+1) - F_2'(K-1) = R_2(K) - P_2(K)$								
	$v'=1$		$v'=2$		$v'=3$		$v'=4$		
K	(1,14)	Olsson	(2,17)	Olsson	(3,17)	(3,19)	Olsson	(4,19)	(4,22)
5	4,87	—	—	—	—	—	—	—	—
7	6,60	—	—	—	—	—	—	—	—
9	8,43	—	—	—	8,13	8,16	—	8,12	8,30
11	10,17	—	—	—	9,81	9,77	—	9,88	9,91
13	11,91	—	—	—	11,54	11,52	—	11,58	11,65
15	13,67	—	—	—	13,21	13,25	13,25	13,33	13,34
17	15,46	15,44	—	—	14,94	14,93	14,97	15,09	15,10
19	17,27	17,22	—	—	16,63	16,66	16,77	16,83	16,76
21	18,98	18,96	—	—	18,33	18,37	18,38	18,51	18,56
23	20,79	20,76	20,33	20,29	20,09	20,11	20,05	20,20	20,24
25	22,47	22,47	22,15	22,15	21,81	21,81	21,80	21,91	21,89
27	24,27	24,30	23,94	23,93	23,59	23,58	23,54	23,59	23,57
29	26,03	26,01	25,69	25,69	25,30	25,34	25,34	25,33	25,33
31	27,80	27,81	27,47	27,36	27,07	27,09	27,08	26,91	26,92
33	29,52	29,53	29,22	29,28	28,78	28,77	28,84	28,49	28,49
35	31,26	31,22	30,92	30,89	30,47	30,51	30,54	30,22	—
37	32,94	32,94	32,65	32,68	32,23	32,26	32,29	—	—
39	34,51	34,51	34,30	34,31	34,01	34,02	33,97	—	—
41	—	35,55	36,02	36,05	35,76	35,79	35,75	—	—
43	—	37,43	37,68	37,76	37,55	37,54	—	—	—
45	—	—	39,36	39,37	39,16	39,25	—	—	—
47	—	—	41,03	40,99	40,87	40,92	—	—	—
49	—	—	42,61	42,59	42,50	42,58	—	—	—
51	—	—	44,18	44,14	44,16	44,02	—	—	—
53	—	—	45,69	45,60	—	—	—	—	—
55	—	—	47,21	—	—	—	—	—	—
57	—	—	48,58	—	—	—	—	—	—
59	—	—	—	—	—	—	—	—	—
61	—	—	—	—	—	—	—	—	—
63	—	—	—	—	—	—	—	—	—
65	—	—	—	—	—	—	—	—	—

Table 16b: The $\Delta_2 F_2'(K)$ values of the vibration level with v'=5,6,7,8

$\Delta_2 F_2'(K) = F_2'(K+1) - F_2'(K-1) = R_2(K) - P_2(K)$							
	$v'=5$		$v'=6$		$v'=7$		$v'=8$
K	(5,22)	(5,23)	(6,23)	(6,25)	(7,25)	(7,27)	(8,27)
3	—	—	—	—	3,20	3,02	2,66
5	—	—	4,63	—	4,73	4,60	4,38
7	—	—	6,23	6,25	6,29	6,32	5,92
9	7,95	7,96	7,97	7,92	7,86	7,99	7,64
11	9,58	9,62	9,66	9,67	9,65	9,71	9,35
13	11,29	11,28	11,34	11,30	11,29	11,25	10,97
15	13,03	12,99	12,99	12,96	12,89	12,94	12,61
17	14,70	14,72	14,67	14,61	14,63	14,63	14,21
19	16,39	16,43	16,25	16,27	16,33	16,28	15,66
21	18,07	18,11	17,90	17,93	17,91	17,97	16,45
23	19,80	19,76	19,54	19,49	19,57	19,57	19,02
25	21,47	21,49	21,08	21,14	21,16	21,18	20,03
27	23,19	23,22	22,68	22,70	22,77	22,79	—
29	24,93	24,93	24,19	24,25	24,34	24,34	—
31	26,65	26,68	25,67	25,72	25,79	25,75	—
33	28,32	28,34	27,08	27,11	—	—	—
35	30,07	30,03	28,44	28,49	—	—	—
37	31,72	31,71	29,74	29,75	—	—	—
39	33,41	33,39	30,94	30,91	—	—	—
41	34,89	34,91	32,04	—	—	—	—
43	35,83	35,84	33,04	—	—	—	—
45	—	—	34,06	—	—	—	—
47	—	—	35,18	—	—	—	—
49	—	—	36,29	—	—	—	—
51	—	—	37,10	—	—	—	—

Table 17a: The $\Delta_2 F_3'(K)$ values of the vibration level with v'=1,2,3,4

$\Delta_2 F_3'(K) = F_3'(K+1) - F_3'(-1) = R_3(K) - P_3(K)$									
	$v'=1$		$v'=2$			$v'=3$		$v'=4$	
K	(1,14)	Olsson	(2,17)	Olsson	(3,17)	(3,19)	Olsson	(4,19)	(4,22)
5	4,53	—	—	—	4,08	—	—	—	—
7	6,14	—	—	—	5,82	—	—	—	—
9	7,81	—	—	—	7,70	—	—	—	—
11	9,59	—	—	—	9,38	—	—	—	—
13	11,40	—	—	—	11,15	11,11	—	11,26	11,30
15	13,15	—	—	—	12,83	12,88	12,84	13,01	12,98
17	14,92	—	15,10	—	14,58	14,61	14,60	14,80	14,72
19	16,72	16,51	16,89	—	16,38	16,36	16,37	16,47	16,46
21	18,41	18,41	18,60	—	18,14	18,08	18,11	18,26	18,25
23	20,06	20,10	20,39	20,33	19,80	19,82	20,14	19,97	19,93
25	21,86	21,81	22,12	22,16	21,58	21,60	21,57	21,47	21,52
27	23,45	23,39	23,86	23,87	23,31	23,37	23,41	23,25	23,12
29	25,07	25,13	25,64	25,55	25,07	25,04	25,12	24,92	24,83
31	26,66	26,73	27,29	27,31	26,72	26,77	26,66	26,70	—
33	28,21	28,21	29,02	28,98	28,41	28,45	28,42	28,24	—
35	29,70	29,77	30,74	30,72	30,08	30,13	30,04	—	—
37	31,25	31,28	32,40	32,38	31,75	31,72	31,74	—	—
39	32,78	32,75	34,06	34,05	33,30	33,31	33,58	—	—
41	34,32	34,28	35,72	35,74	34,82	34,90	34,85	—	—
43	—	—	37,29	37,30	36,25	36,31	—	—	—
45	—	—	38,85	38,90	37,68	37,68	—	—	—
47	—	—	40,39	40,35	39,25	39,07	—	—	—
49	—	—	41,83	41,81	—	—	—	—	—
51	—	—	43,22	43,21	—	—	—	—	—
53	—	—	44,72	44,50	—	—	—	—	—

Table 17b: The $\Delta_2 F_3'(K)$ values of the vibration level with v'=5

$\Delta_2 F_3'(K) = F_3'(K+1) - F_3'(K-1) = R_3(K) - P_3(K)$									
	$v'=5$			$v'=5$			$v'=5$		
K	(5,22)	(5,22)	K	(5,22)	(5,22)	K	(5,22)	(5,22)	
7	5,78	—	21	17,78	17,77	35	29,00	29,01	
9	7,46	—	23	19,44	19,46	37	30,43	30,41	
11	9,12	9,13	25	21,16	21,09	39	31,77	31,76	
13	10,86	10,89	27	22,77	22,85	41	33,04	33,10	
15	12,61	12,63	29	24,39	24,41	43	—	34,42	
17	14,29	14,32	31	25,97	25,99	45	35,65	35,69	
19	16,09	16,05	33	27,54	27,49	47	37,10	37,09	

Table 18: The $\Delta_2 F_i''(K)$ values of the vibration level with v"=17

	$\Delta_2 F_i''(K) = F_i''(K+1) - F_i''(K-1) = R_i(K-1) - P_i(K+1)$					
	$\Delta_2 F_1''(K)$		$\Delta_2 F_2''(K)$		$\Delta_2 F_3''(K)$	
K	(2,17)	(3,17)	(2,17)	(3,17)	(2,17)	(3,17)
4	—	5,58	—	—	—	4,08
6	—	7,73	—	—	—	6,18
8	—	9,77	—	9,15	—	8,30
10	—	11,89	—	11,25	—	10,67
12	—	13,89	—	13,41	—	12,93
14	—	16,00	—	15,55	—	14,90
16	—	17,97	17,73	17,68	—	17,14
18	—	20,18	19,83	19,76	19,37	19,35
20	—	22,28	21,82	21,85	21,49	21,55
22	—	24,36	24,11	24,02	23,66	23,69
24	—	26,43	26,16	26,18	25,92	25,80
26	—	28,54	28 34	28,32	28,02	27,96
28	30,63	30,67	30,44	30,41	30,17	30,18
30	32,78	32,80	32,56	32,56	32,31	32,33
32	34,89	34,89	34,70	34,71	34,48	34,44
34	37,01	37,03	36,76	36,75	36,65	36,62
36	39,12	39,10	39,00	38,90	38,81	38,75
38	41,21	41,22	41,05	41,08	40,94	40,91
40	43,36	43,31	43,20	43,20	43,10	43,09
42	45,47	45,43	45,30	45,40	45,18	45,12
44	47,58	47,56	47,46	47,41	47,33	47,22
46	49,71	49,70	49,55	49,52	49,45	49,48
48	51,78	51,78	51,73	51,66	—	51,79
50	53,85	53,87	53,84	53,76	—	54,01
52	56,06	55,97	55,91	56,03	—	56,17
54	58,10	58,10	58,01	58,13	—	—
56	60,21	60,19	60,17	—	—	—
58	62,30	62,30	62,19	—	—	—
60	64,42	64,43	64,30	—	—	—
62	66,54	66,52	—	—	—	—
64	68,42	—	—	—	—	—
66	70,66	—	—	—	—	—

Table 19: The $\Delta_2 F_i''(K)$ values of the vibration level with v"=19

	$\Delta_2 F_i''(K) = F_i''(K+1) - F_i''(K-1) = R_i(K-1) - P_i(K+1)$					
	$\Delta_2 F_1''(K)$		$\Delta_2 F_2''(K)$		$\Delta_2 F_3''(K)$	
K	(3,19)	(4,19)	(3,19)	(4,19)	(3,19)	(4,19)
6	7,84	—	—	—	—	—
8	9,66	—	8,79	9,14	—	—
10	11,71	11,75	11,08	11,14	—	—
12	13,78	—	13,20	13,10	12,58	12,63
14	15,77	15,71	15,31	15,28	14,77	14,85
16	17,89	17,86	17,45	17,41	16,96	17,04
18	19,96	19,95	19,54	19,56	19,07	19,08
20	21,99	21,94	21,65	21,61	21,27	21,29
22	24,06	24,05	23,75	23,80	23,38	23,44
24	26,16	26,14	25,86	25,81	25,49	25,49
26	28,22	28,20	27,91	27,94	27,67	27,66
28	30,36	30,36	30,09	30,04	29,79	29,77
30	32,41	32,37	32,18	32,18	31,98	31,98
32	34,48	34,48	34,33	34,30	34,06	34,11
34	36,57	36,57	36,35	36,40	36,19	36,11
36	38,66	38,65	38,43	38,43	38,30	—
38	40,72	40,71	40,59	40,57	40,41	—
40	42,82	42,79	42,70	42,66	42,56	—
42	44,91	44,83	44,82	44,83	44,67	—
44	47,00	46,95	46,91	—	46,71	—
46	49,06	49,07	49,00	—	48,87	—
48	51,21	51,09	51,09	—	50,96	—
50	53,27	53,34	53,15	—	—	—
52	55,39	—	55,23	—	—	—
54	57,35	57,25	—	—	—	—
56	59,50	—	—	—	—	—
58	61,51	—	—	—	—	—

Table 20: The $\Delta_2 F_i''(K)$ values of the vibration level with v"=22

$\Delta_2 F_i''(K) = F_i''(K+1) - F_i''(K-1) = R_i(K-1) - P_i(K+1)$						
	$\Delta_2 F_1''(K)$		$\Delta_2 F_2''(K)$		$\Delta_2 F_3''(K)$	
K	(4,22)	(5,22)	(4,22)	(5,22)	(4,22)	(5,22)
6	—	7,53	—	6,50	—	—
8	9,55	—	8,95	—	—	—
10	11,50	11,51	10,88	10,89	—	—
12	13,40	13,49	12,88	12,98	12,28	12,32
14	15,50	15,57	15,03	15,02	14,52	14,47
16	17,53	17,53	17,15	17,15	16,60	16,56
18	19,54	19,56	19,12	19,19	18,74	18,75
20	21,68	21,62	21,28	21,25	20,89	20,86
22	23,61	23,66	23,33	23,31	22,89	22,94
24	25,68	25,68	25,39	25,38	25,12	25,06
26	27,75	27,70	27,43	27,42	27,21	27,17
28	29,79	29,77	29,45	29,49	29,31	29,21
30	31,78	31,79	31,52	31,63	31,20	31,30
32	33,79	33,80	33,66	33,61	—	33,41
34	35,94	35,87	35,71	35,74	—	35,47
36	37,88	37,90	—	37,74	—	37,60
38	39,97	39,96	—	39,86	—	39,63
40	42,10	42,07	—	41,91	—	41,77
42	43,95	43,97	—	43,93	—	—
44	—	46,08	—	46,02	—	45,92
46	—	48,18	—	—	—	47,97
48	—	50,26	—	—	—	49,99
50	—	52,21	—	—	—	—
52	—	54,30	—	—	—	—

Table 21: The $\Delta_2 F_i''(K)$ values of the vibration level with v"=23

$\Delta_2 F_i''(K) = F_i''(K+1) - F_i''(K-1) = R_i(K-1) - P_i(K+1)$					
	$\Delta_2 F_1''(K)$		$\Delta_2 F_2''(K)$		$\Delta_2 F_3''(K)$
K	(5,23)	(6,23)	(5,23)	(6,23)	(5,23)
6	7,36	—	—	6,74	—
8	9,31	9,44	—	8,71	—
10	11,38	11,44	10,84	10,83	10,17
12	13,44	13,36	12,89	12,97	12,28
14	15,45	15,52	14,92	14,90	14,33
16	17,45	17,45	17,01	17,03	16,51
18	19,46	19,53	19,08	10,95	18,59
20	21,51	21,49	21,14	21,13	20,68
22	23,52	23,46	23,20	23,16	22,82
24	25,57	25,59	25,20	25,20	24,85
26	27,58	27,54	27,27	27,24	27,03
28	29,55	29,49	29,34	29,35	29,05
30	31,62	31,63	31,41	31,37	31,06
32	33,65	33,64	33,46	33,38	33,15
34	35,68	35,71	35,48	35,45	35,28
36	37,74	37,72	37,40	37,48	37,32
38	39,74	39,75	39,56	39,62	39,40
40	41,76	41,78	41,63	41,62	41,48
42	43,77	43,80	43,69	43,62	43,66
44	45,83	45,83	45,74	45,67	45,63
46	47,95	47,93	—	47,69	47,59
48	49,91	49,96	—	49,89	—
50	51,86	—	—	51,78	—
52	53,97	—	—	—	—

Table 22: The $\Delta_2 F_1''(K)$ values of the vibration level with v"=25

$\Delta_2 F_i''(K) = F_i''(K+1) - F_i''(K-1) = R_i(K-1) - P_i(K+1)$				
	$\Delta_2 F_1'(K)$		$\Delta_2 F_2''(K)$	
K	(6,25)	(7,25)	(6,25)	(7,25)
4	—	—	4,54	4,48
6	—	—	6,57	6,54
8	—	—	8,63	8,62
10	—	—	10,66	10,67
12	—	—	12,73	12,71
14	15,25	15,19	14,70	14,73
16	17,23	17,22	16,81	16,73
18	19,18	—	18,80	18,81
20	21,19	21,18	20,85	20,87
22	23,19	23,21	22,85	22,89
24	25,24	25,20	24,90	24,93
26	27,13	27,19	26,95	26,85
28	29,22	29,21	29,00	28,95
30	31,21	31,19	31,00	31,02
32	33,26	33,23	33,02	33,02
34	35,23	35,26	35,02	34,97
36	37,24	37,23	37,07	37,04
38	39,20	39,12	39,05	—
40	41,21	40,98	41,06	—
42	—	43,20	—	—

Table 23: The $\Delta_2 F_1''(K)$ values of the vibration level with v"=27

$\Delta_2 F_i''(K) = F_i'(K+1) - F_i'(K-1) = R_i(K-1) - P_i(K+1)$				
	$\Delta_2 F_1'(K)$		$\Delta_2 F_2'(K)$	
K	(7,27)		(7,27)	(8,27)
2	—		2,54	—
4	—		4,60	4,72
6	—		6,53	6,61
8	—		8,62	8,60
10	—		10,62	10,58
12	12,81		12,52	12,47
14	15,13		14,52	14,53
16	17,05		16,56	16,60
18	18,92		18,58	18,57
20	20,91		20,60	20,61
22	22,97		22,60	22,58
24	24,84		24,58	24,57
26	26,87		26,56	26,54
28	28,84		28,58	—
30	30,79		30,58	—
32	32,80		—	—
34	34,78		—	—
36	36,74		—	—
38	38,62		—	—

IV. The determination of the K values and the molecular constants

From equations (1), (9) and (10) it follows that

$$\Delta_2 F'_2(K) = F'_2(K+1) - F_2(K-1)$$

$$= B'_v(K+1)(K+2) + D'_v(K+1)^2(K+2)^2 - B_v(K-1)K - D'_v(K-1)^2K^2$$

$$= 4B'_v(K+\tfrac{1}{2}) + 8D'_v(K+\tfrac{1}{2})^3. \qquad (15)$$

Equation (9) was chosen here because in it f_2 is independent of K and therefore vanishes in $\Delta_2 F'_2(K)$. Since D'_v is usually very small in comparison to B'_v, the term with D'_v can be neglected for smaller values of K. A similar equation also holds for $\Delta_2 F''_2(K)$.

The $\Delta_2 F'_2(K)$ values of Tables 15, 16 and 17 and the $\Delta_2 F''_2(K)$ values of Tables 18, 19, 20, 21, and 22 can now be graphed with respect to K. From the slope of these curves it is possible to compute B'_v for the vibration levels with v'=1, 2, 3, 4, 5, 6, 7 and 8 and B''_v for the vibration levels with v"=17, 19, 22, 23, 25 and 27. From Tables 2 and 3 can also be drawn the $\Delta_2 F''_2(K)$ values for the vibration level with v"=14, and from these values the B''_v values can be determined as above. As will be mentioned again below, every other line of the branches is missing, and therefore the graphically determined slope according to equation 15 must be divided by 8 to obtain the correct value of B_v. These values of B'_v and B''_v are given in Table 24 together with B'_8, B'_7 and B''_0 values drawn from an unpublished work by Wilson[10]. An extract from this work was most generously sent to me by Prof. G. Herzberg of the physics department of the University of Saskatchewan, Saskatoon, Canada. The B''_2, B''_3 and B''_4 values given in Table 24 are drawn from the work of Olsson. The B'_1, B'_2 and B'_3 values given by Olsson are 0.2173, 0.2174 and 0.2176 cm^{-1}. It can be seen from this that the B'_1 value of Olsson is quite different from that calculated here. Therefore Olsson's $\Delta_2 F'_2(K)$ values for v'=1, 2 and 3 were entered graphically, and the values of B'_1, B'_2 and B'_3 resulting from this are given in Table 24.

Table 24: The molecular constants

v''	B_v''	B_e'', r_e'', α_e'' und D_e''
27	0,2503 ± ,0001 (Naudé)	—
25	0,2539 ± ,0001 „	—
24	0,2556 ± ,0001 „	—
23	0,2568 ± ,0001 „	—
22	0,2589 ± ,0001 „	—
19	0,2633 ± ,0001 „	—
18	0,2651 ± ,0001 „	— (1)
17	0,2666 ± ,0002 „	B_0'' (extrapoliert) = 0,2947 cm^{-1}
16	0,2681 ± ,0001 „	—
15	0,2700 ± ,0001 „	B_e'' = 0,2956 cm^{-1}
14	0,2716 ± ,0001 „	—
8	0,2819 ± ,0002 (Wilson)	r_e'' = 1,893 × 10^{-8} cm
7	0,2834 ± ,0002 „	—
4	0,2883 ± ,0002 (Olsson)	α_e'' = 0,0016 cm^{-1}
3	0,2896 ± ,0002 „	—
2	0,2915 ± ,0001 „	D_e'' = — 19,6 × 10^{-8} cm^{-1}

v'	B_v'	B_e', r_e', α_e' und D_e'
7	0,2085 ± ,0002 (Naudé)	—
6	0,2102 ± ,0001 „	—
5	0,2102 ± ,0001 „	—
4	0,2150 ± ,0001 „	B_e' = 0,2219 cm^{-1}
3	0,2129 ± ,0001 „ (2)	—
3	0,2136 (Olsson nachgerechnet)	r_e' = 2,184 × 10^{-8} cm
2	0,2175 ± ,0001 (Naudé) (2)	—
2	0,2177 (Olsson nachgerechnet)	α_e' 0,0018 cm^{-1}
1	0,2205 ± ,0001 (Naudé) (2)	—
1	0,2200 (Olsson nachgerechnet)	D_e' = — 23,1 × 10^{-8} cm^{-1}
0	0,221 ± ,001 (Wilson)	—

Key: (1) Extrapolated; (2) recomputed.

B_e, α_e and r_e can be calculated from the following equations:

$$\alpha_e = (B_o - B_v)/v$$

$$B_e = B_o + \tfrac{1}{2}\alpha_v$$

$$r_e^2 = \frac{27.994 \cdot 10^{-40}}{\mu B_e} \quad \text{where} \quad \frac{1}{\mu} = \frac{1}{32.06} + \frac{1}{32.06}.$$

32.06 was taken to be the atomic weight of the most common isotope of sulfur. D_e was calculated from the equation

$$D_e = -4\frac{B_e^3}{\omega_e^2} .$$

According to Wilson, ω_e''=725.68±.01 cm^{-1}. It is impossible to determine ω_e' precisely, because of the distortions in the higher state. Following the analysis of Fowler and Vaidya, ω_e' can be assumed to be about 435 cm^{-1}.

The precise values of the rotation quantum numbers K could also be determined from the curves cited above by extrapolation

of the curves of equation (15) to $\Delta_2 F_2(K)=0$. If the K values are correctly correlated, it is found that the straight-line curve intersects the K axis at $K=-\frac{1}{2}$. It can be seen from this that the rotation levels with even K values are absent in the lower state, while the odd K values are missing in the upper state. Since every other level is absent, the conclusion may be drawn that the S^{32} atom has no nuclear spin.

Similar results were obtained for the Schumann-Runge bands by Ossenbrüggen and by Lochte-Holtgreven and Dieke. Mulliken[11] showed that the lower state of O_2 was in all probability a $^3\Sigma_g^-$ state. From this it is possible to conclude that the analogous S_2 bands are to be ascribed to a $^3\Sigma_u^- \rightarrow ^3\Sigma_g^-$ transition. Figure 3 gives a schematic representation of the S_2 rotation levels.

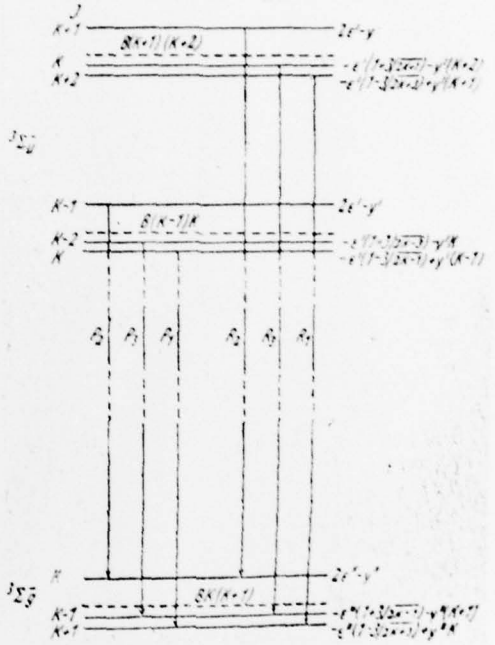


Figure 3: S_2 level diagram

V. Discussion of results

From Tables 15a, 16a and 17a it can be seen that the spectral branches can be traced to lower and higher quantum numbers in emission than was possible in the absorption analysis of Olsson. Furthermore, the $\Delta_2 F_1(K)$ values here show better agreement than the values drawn from the work of Olsson, which doubtless stems from the fact that the lines are more precisely measurable in emission than in absorption.

It is notable that the branches of the (2.17) band could not be traced down to the smaller K values, although the combinations for the v"=17 level were known precisely from the analysis of the (3.17) band. This situation must probably be ascribed to distortions. In the (4.19) and (4.22) bands the R_3

and P_3 branches are weak, and in the (6.23), (6.25), (7.25) and (7.27) bands these branches could not be found at all, while in the (8.27) band only the R_2 and P_2 branches were found. It is possible that these irregularities are to be ascribed to distortions, and are connected with the predissociation of the S_2 molecule. According to Herzberg, this predissociation occurs in the v'=10 level. Initially it was also a purpose of this work to attempt to clarify these disturbances, and in fact photographs were made, measured and investigated of the (8.29) and (9.29) bands, but with no further success than that a few lines of the R_2 and P_2 series were found in the (8.29) band.

The experimental portion of the present work was performed in the Merensky Institute of Physics at the University of Stellenbosch (South Africa).

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